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# New models for PIXE simulation with Geant4

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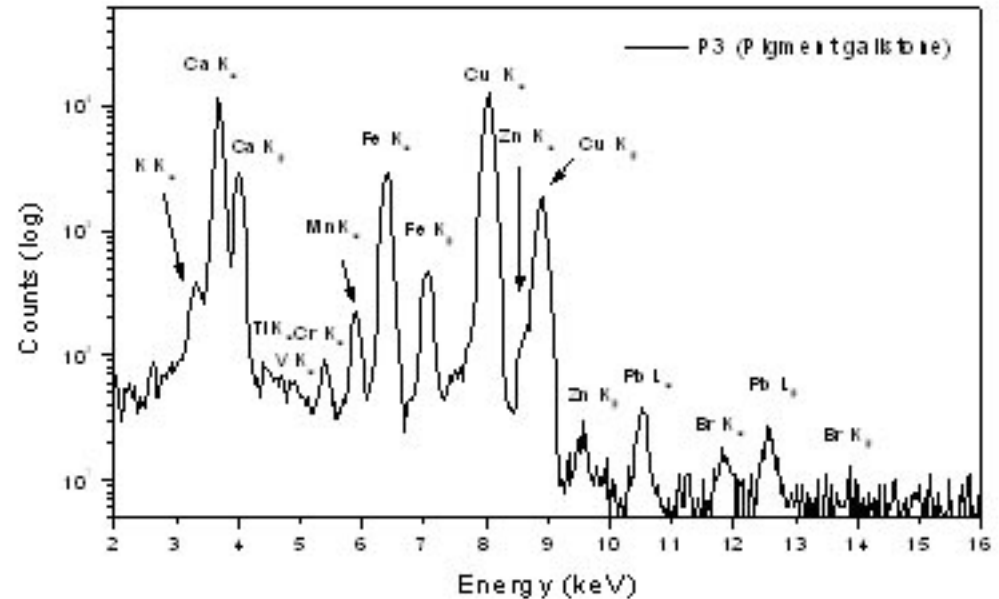
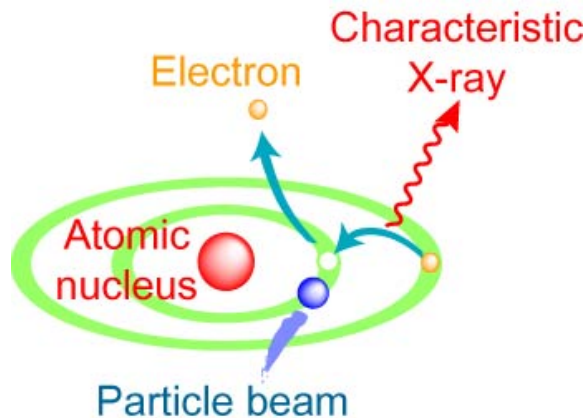
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# PIXE

## Particle Induced X-ray Emission

Particle = proton, ion (electron)



The physics of PIXE is simple

The simulation of PIXE is **NOT** simple

# PIXE simulation recipe

## Ingredients

- Proton (ion) **ionisation cross sections** for individual shells
- Radiative and non-radiative **transition probabilities**
- Atomic **binding energies** (X-ray energies)

## Instructions

- **Create a vacancy** in the shell occupancy due to ionisation
- **De-excite** the atom through fluorescence and Auger emission

## A touch of spice

**Infrared divergence** of the cross section for  $\delta$ -ray emission

Monte Carlo codes neutralize the spice by introducing “**cuts**”  
(i.e. a threshold for  $\delta$ -ray production)  
Below the threshold: ionisation treated as *continuous energy loss*  
Above the threshold: *emission of an electron*

PIXE is and intrinsically **discrete** process, which is intimately associated with a **continuous-discrete** one

## Note

One of the ingredients (ionisation cross sections) is available in limited quantity (for a few **inner shells only**)

# PIXE in Geant4 (and other codes)

- **Specialized codes for PIXE analysis (and simulation)**
  - GeoPIXE, GUPIX, PIXAN, PixeKLM, Sapix, WinAxil, Wits-HEX etc.
  - Only concerned with experimental observables relevant to material analysis
- **Impact ionisation by electrons**
  - EGS\*, Penelope
  - Cross sections available for all shells
  - “independent” discrete process + “regular” continuous-discrete ionisation
  - Penelope literature reports cases of negative energy deposits in volumes subject to large fluctuations
- **Geant4 struggle with PIXE started in 2001**
- **It is still an open issue, that motivated a new R&D project**
  - Not just on PIXE, but on fundamental methods of particle transport...

# PIXE history in Geant4

## Geant4 Low Energy Electromagnetic package

- No PIXE in the first implementation of hadron/ion ionisation
  - total ionisation cross section as in Phys. Ref. Manual (M. Maire & L. Urban, Geant4 Standard EM)
- PIXE embedded in hadron ionisation process
- Design to handle multiple shell cross section models (MGP)

### Shell ionisation cross section models used by G4hLowEnergyIonisation

- **Gryzinski model**
    - Shell ionisation cross sections,  $1 \leq Z \leq 92$ , all shells as in EADL
    - *Implementation: S. Dussoni, V. Ivanchenko, A. Mantero, S. Saliceti, 2001-2004*
  - **Fit to H. Paul's K-shell experimental database**
    - Shell ionisation cross sections,  $4 \leq Z \leq 92$
    - *Implementation: A. Mantero, S. Saliceti, 2004*
  - **Refined fit to H. Paul's K-shell experimental database**
    - Shell ionisation cross sections,  $4 \leq Z \leq 92$
    - *Implementation: A. Mantero, S. Saliceti, 2004-2005*
- PostStepDolt*  
*+ undocumented model in AlongStepDolt*

### Shell ionisation cross section models, not used by any process

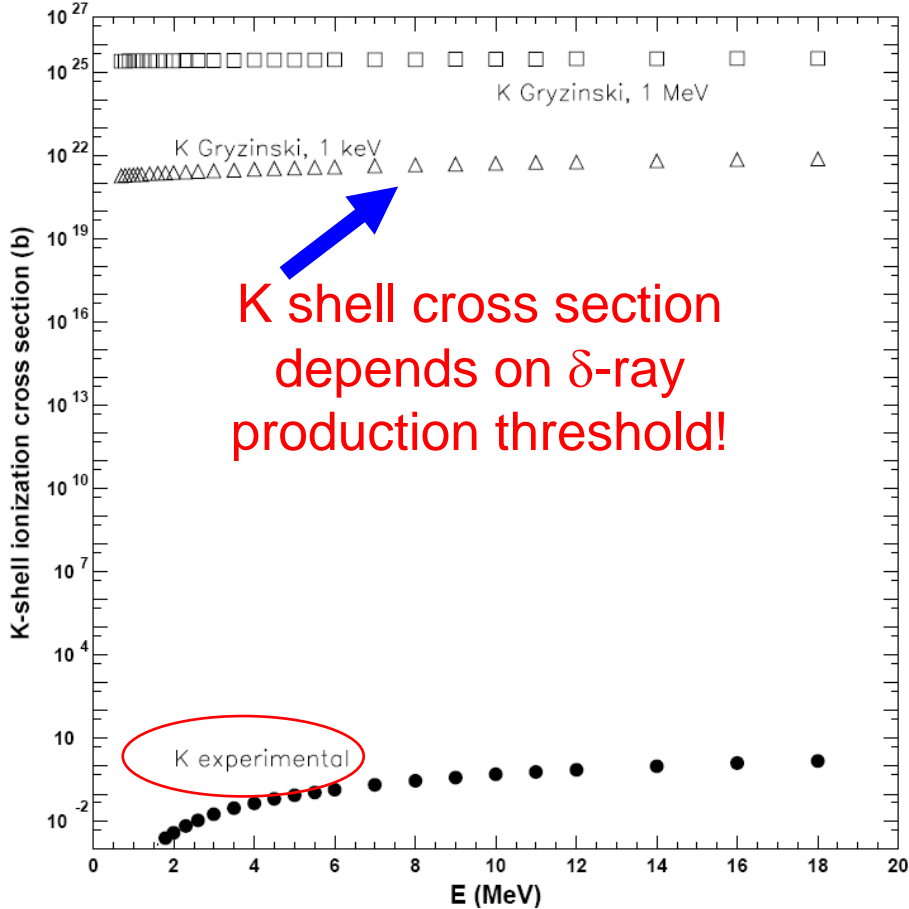
- **ECPSSR (K), semi-empirical (L), interpolation of H. Paul's data (K-shell)**
  - *Implementation: H. Ben Abdelouahed, Geant4 9.2, 2008*
  - *NIM B paper H. Abdelhouahed, S. Incerti, A. Mantero, Jan 2009*

## Geant4 R&D project, THIS TALK... and a 40 page paper

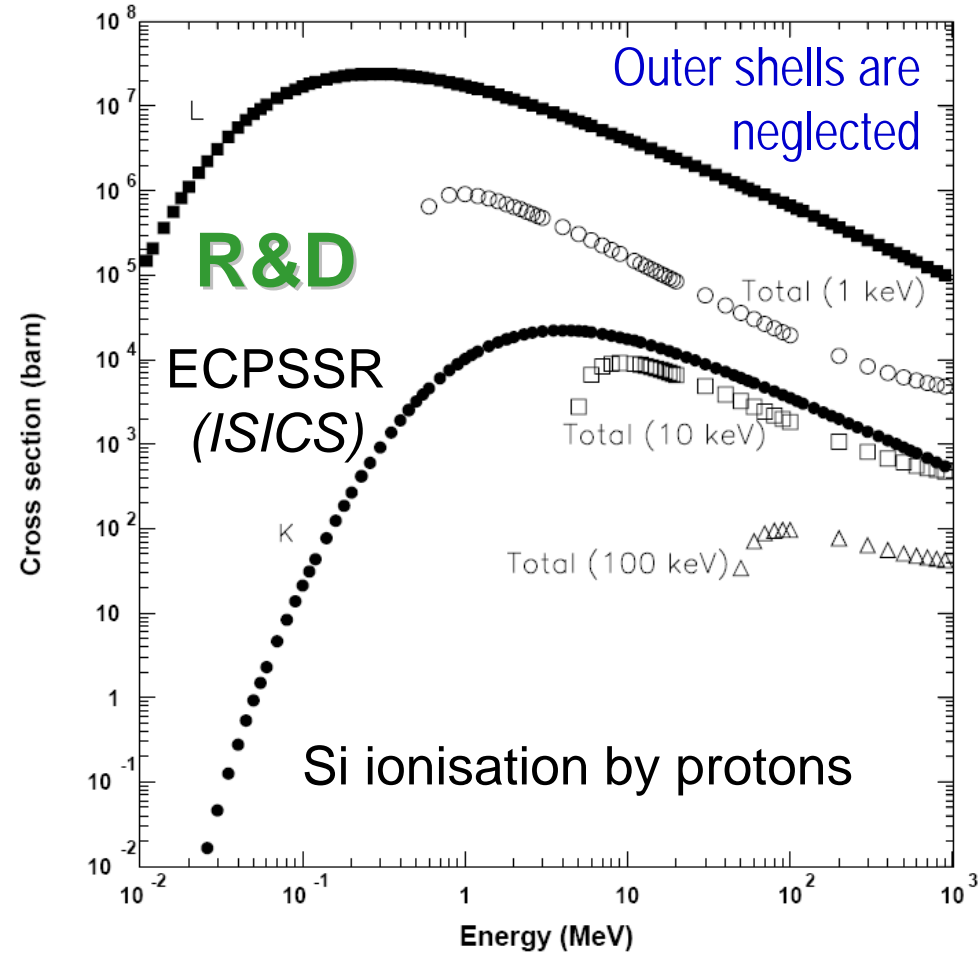
- Part of a R&D project to address fundamental concepts in particle transport

# First Geant4 PIXE development cycle

Wrong: theory or software or both?



+ implementations based on fits to empirical database (correct!)



Depending on the  $\delta$ -ray production cut, the “total” cross section may be smaller than the **K shell** ionisation cross section

# Pixe in Geant4 9.2

New Geant4 cross section models for PIXE simulation

H. Ben Abdelouahed<sup>a,\*</sup>, S. Incerti<sup>b</sup>, A. Mantero<sup>c</sup>

Nuclear Instruments and Methods in Physics Research B 267 (2009) 37–44

- ECPSSR theoretical (K, p- $\alpha$ )
- Paul&Sacher, Paul&Bolik empirical (K, p- $\alpha$ )
- Orlic et al. semi-empirical (L, p)

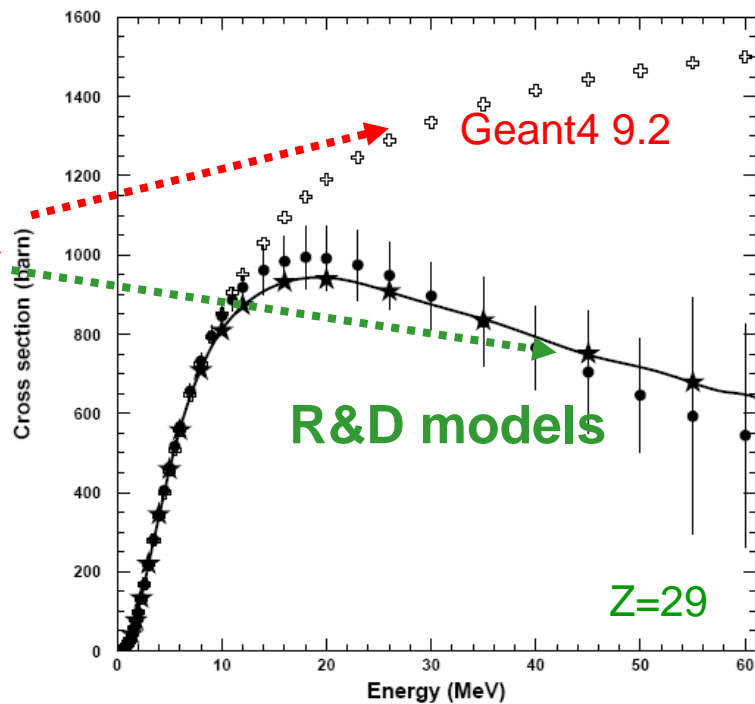
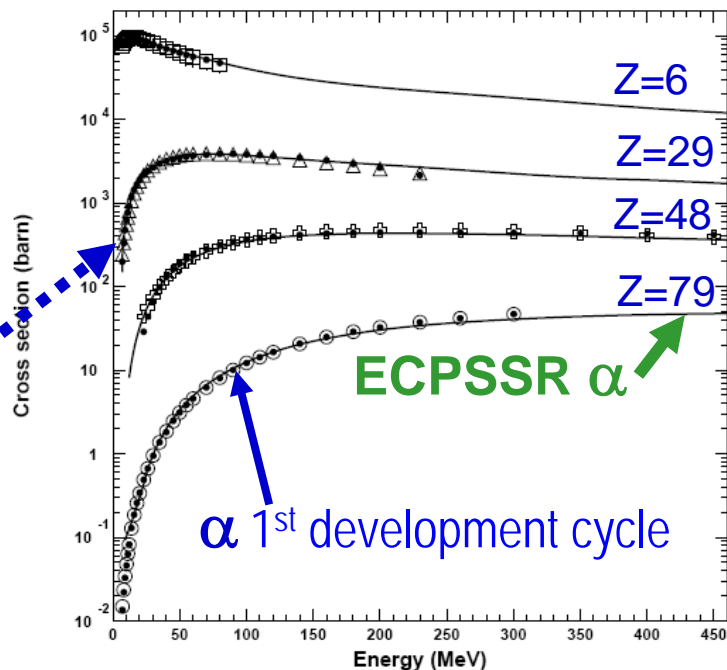
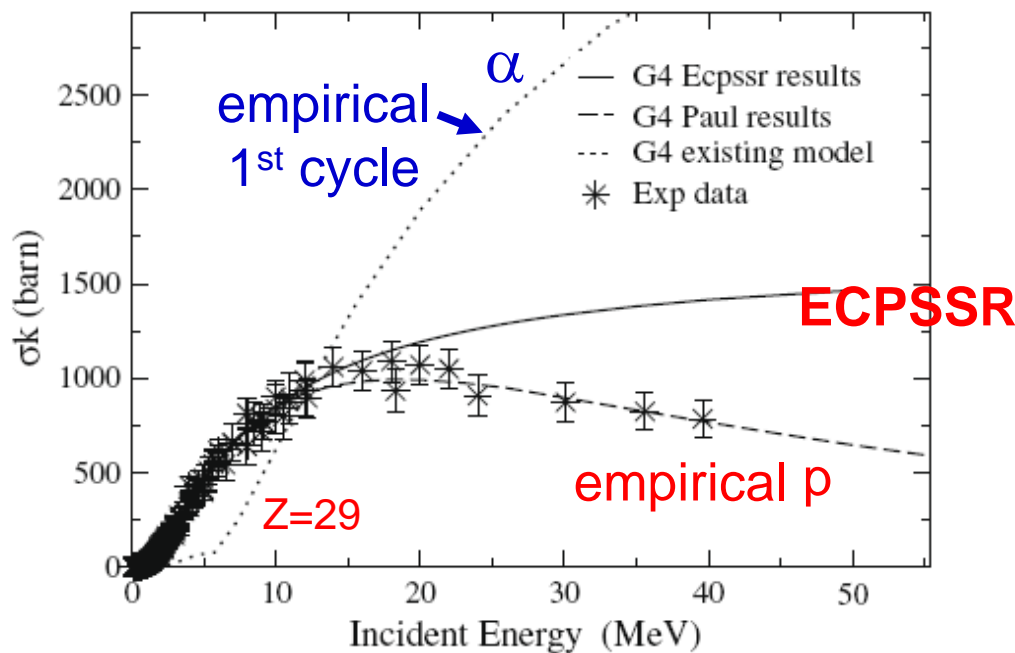


Fig. 2. K-shell ionization cross section by protons impact of element  $Z_2 = 29$ .

# Geant4 9.2 performance

ECPSSR model, K shell, protons			
Element	Geant4 9.2	This work	Speed Gain Factor
Si	3.86	0.62	5.9
Cu	3.96	0.63	6.3
Cd	4.24	0.62	6.8
Au	5.21	0.64	8.1
Empirical model, K shell, protons			
Element	Geant4 9.2	This work	Speed Gain Factor
Si	112.83	0.63	179
Cu	107.58	0.62	173
Cd	78.68	0.59	133
Au	66.21	0.53	125
Empirical model, K shell, $\alpha$ particles			
Element	Previous Geant4	Geant4 9.2	This work
Si	1.93	119.64	1.21
Cu	1.89	108.82	1.16
Cd	1.89	103.14	1.08
Au	1.77	85.22	0.82

Complex theoretical calculations  
(6-8 times slower)

2 orders of magnitude slower  
than R&D models

~50 times slower than  
previous Geant4 model for  $\alpha$   
with same functionality

...and much more



# Still a long way to go...

Can we deal with PIXE correctly?

## Short term R&D

- Up to where can one go with existing instruments?

Do we know how to deal with PIXE correctly?

## Long term R&D

- Part of a larger R&D study on transport methods in simulation
- See talk in Core Tools session on Thursday at 2 pm

PIXE is a physically interesting playground

...but the issue is the

interplay of **continuous** and **discrete transport methods**

Nanotechnology  
detectors

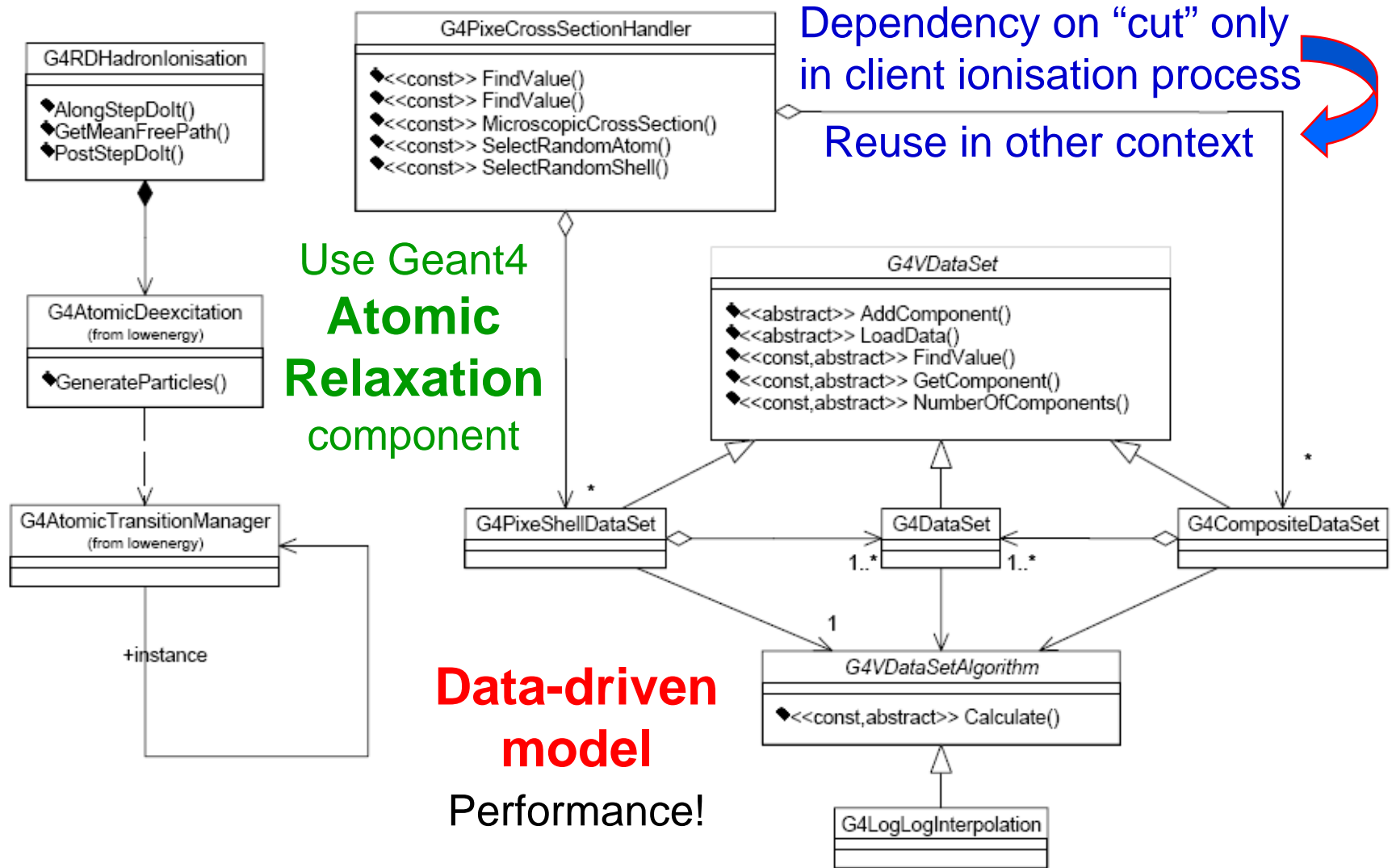
Radiation effects  
to components

LHC  
RADMON

Gaseous  
detectors

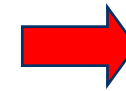
# Crisp domain decomposition

No dependence of PIXE component on  $\delta$ -ray production threshold



# Ionisation cross sections

■ Theoretical  
■ Empirical



To be released  
as a data library



Thanks to RSICC!

*Theoretical cross  
 sections tabulated by  
 ISICS  
 (thanks to S. Cipolla!)*

Subject to  
 rigorous  
**experimental  
 validation**

## Protons, K shell

Model	Z range
ECPSSR	6-92
ECPSSR High Energy	6-92
ECPSSR Hartree-Slater	6-92
ECPSSR United Atom	6-92
ECPSSR reference [38]	6-92
PWBA	6-92
Paul and Sacher	6-92
Kahoul et al.	6-92

## Protons, L shell

Model	Z range
ECPSSR	6-92
ECPSSR United Atom	6-92
PWBA	6-92
Miyagawa et al.	40-92
Orlic et al.	43-92
Sow et al.	43-92

## Protons, M shell

Model	Z range
ECPSSR	6-92
ECPSSR United Atom	6-92
PWBA	6-92

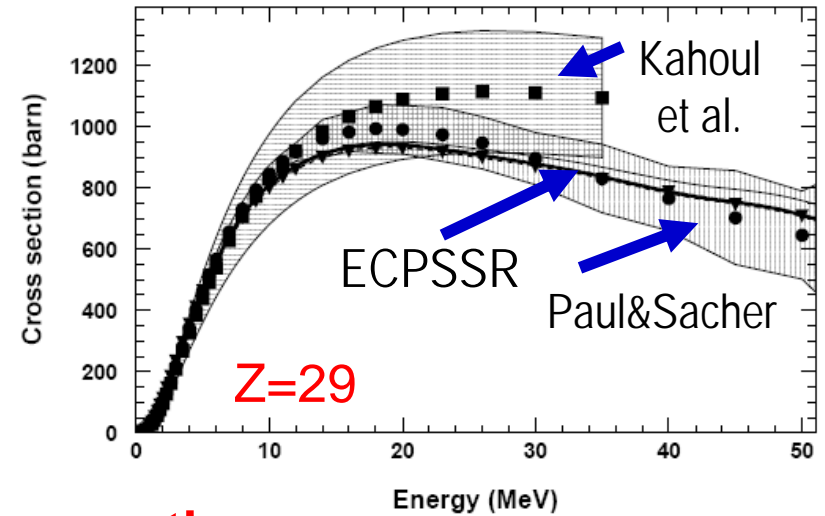
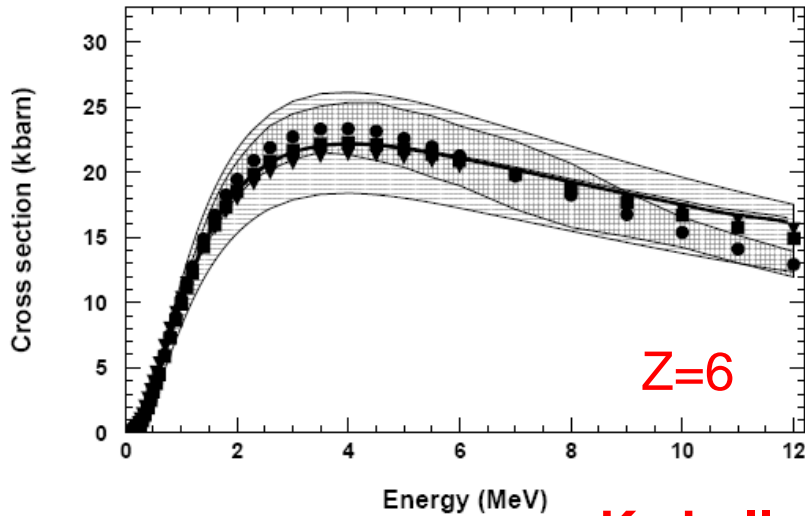
## $\alpha$ , K shell

Model	Z range
ECPSSR	6-92
ECPSSR Hartree-Slater	6-92
ECPSSR United Atom	6-92
ECPSSR reference [39]	6-92
PWBA	6-92
Paul and Bolik	6-92

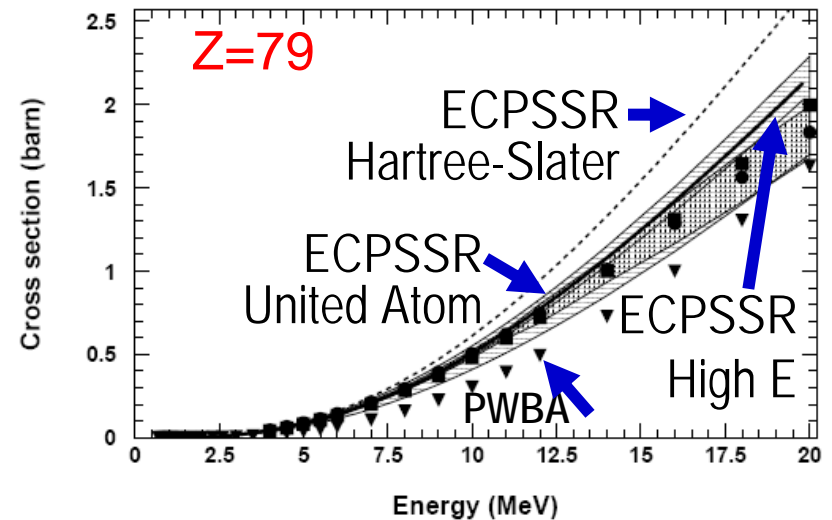
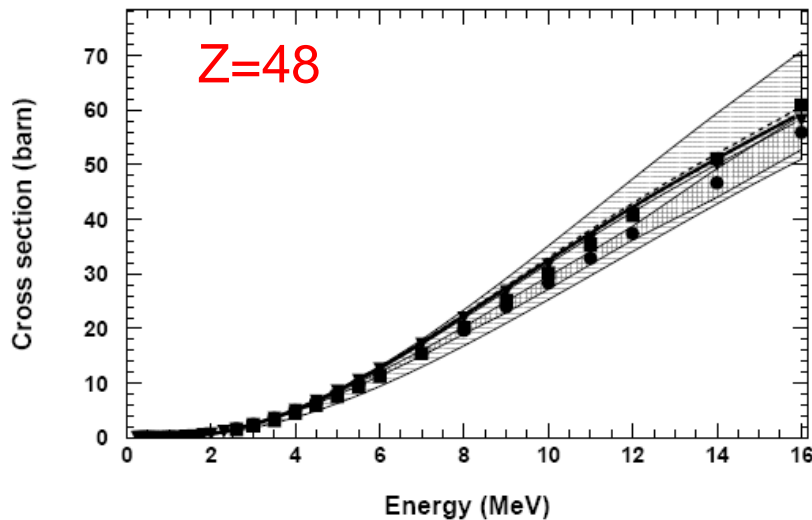
## $\alpha$ , L and M shell

Model	Z range
ECPSSR	6-92
ECPSSR United Atom	6-92
PWBA	6-92

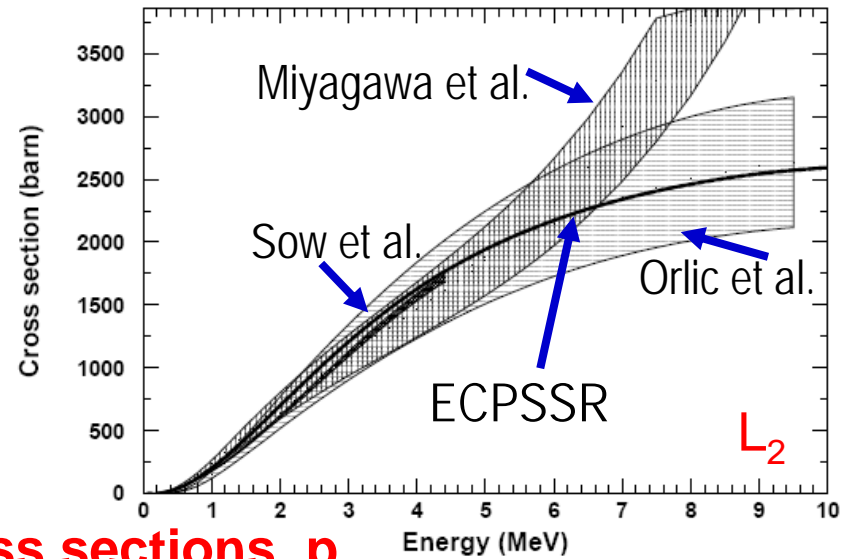
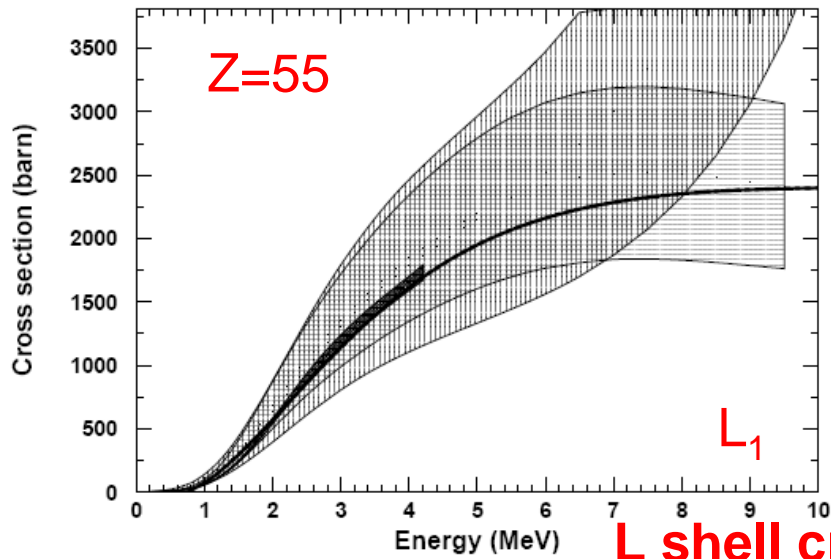
# Similarities and differences, K



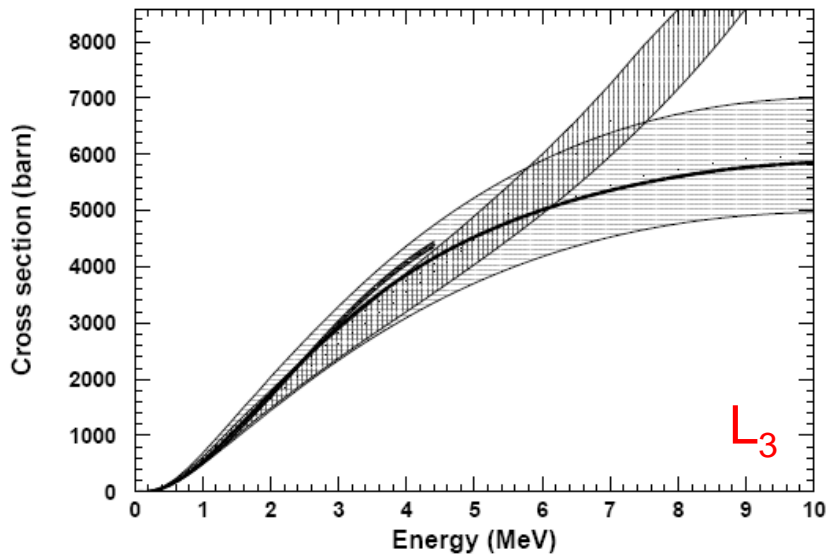
## K shell cross sections, p



# Similarities and differences, L



**L shell cross sections, p**

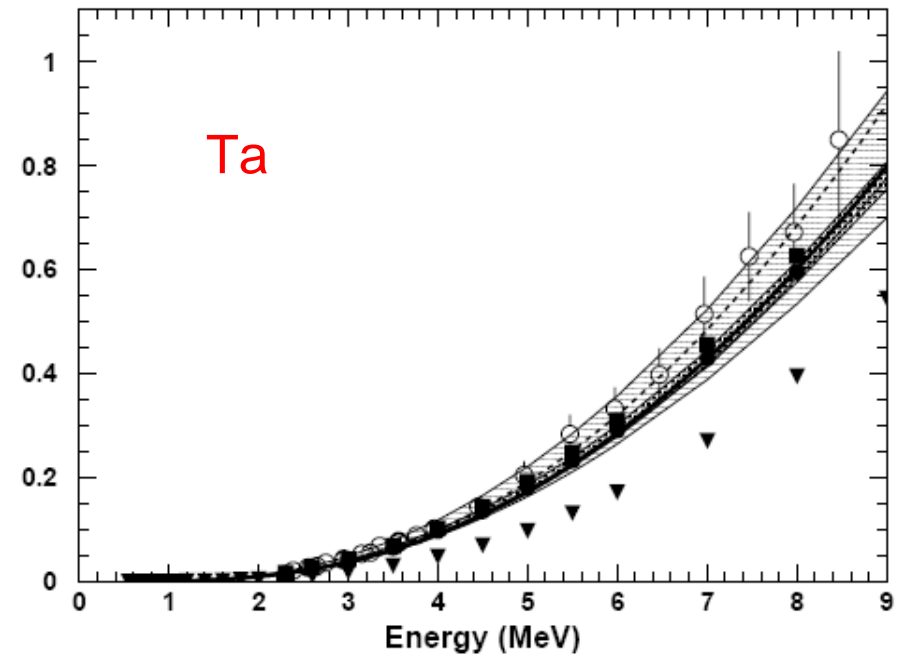
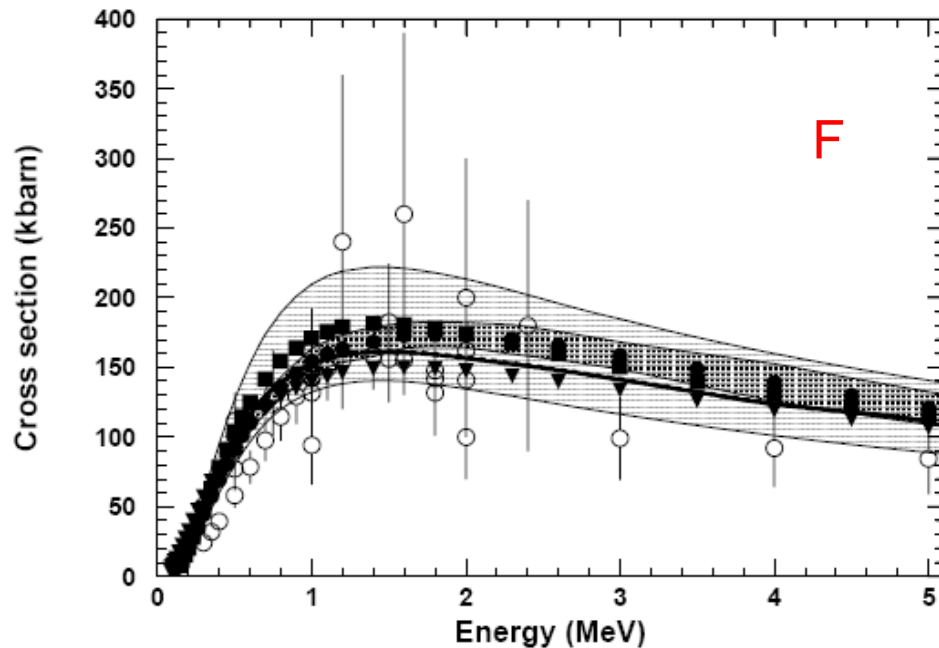


No systematic, quantitative analysis of all the existing theoretical and empirical models documented in literature

# Experimental validation, K shell

Experimental data from  
Paul & Sacher  
compilation

Cross section (barn)



**Ionisation** cross sections

**X-ray production** cross sections

$$\sigma_i = \sigma_X / \omega_K$$

# $\chi^2$ test: p-values

## K shell, protons

Z	ECPSSR	ECPSSR HE	ECPSSR HS	ECPSSR UA	Paul Sacher	Kahoul et al.
6	0.200	0.203	0.490	0.200	0.998	0.989
7	0.057	0.061	0.246	0.057	0.818	0.806
8	0.906	0.910	0.922	0.906	0.981	0.971
9	0.147	0.136	0.124	0.147	0.029	0.012
10	0.044	0.046	0.083	0.044	0.791	0.171
60	0.296	0.185	0.550	0.296	0.385	< 0.001
62	0.049	0.029	0.642	0.049	0.570	< 0.001
65	0.322	0.161	0.928	0.322	0.310	0.523
67	< 0.001	< 0.001	0.844	< 0.001	0.012	0.001
69	0.003	0.004	0.078	0.003	0.741	< 0.001
73	0.013	0.002	0.946	0.013	0.193	0.998
90	< 0.001	< 0.001	0.001	< 0.001	< 0.001	< 0.001

P-VALUES FROM THE  $\chi^2$  TEST COMPARING K SHELL IONIZATION CROSS SECTIONS FOR PROTONS AGAINST EXPERIMENTAL DATA  $\sigma_{i,X,A}$

Z	ECPSSR	ECPSSR HE	ECPSSR HS	ECPSSR UA	Paul Sacher	Kahoul et al.	Z	ECPSSR	ECPSSR HE	ECPSSR HS	ECPSSR UA	Paul Sacher	Kahoul et al.
6	0.797	0.818	0.959	0.797	< 0.001	< 0.001	40	0.045	0.066	0.102	0.039	0.208	0.044
7	< 0.001	< 0.001	0.063	< 0.001	< 0.001	< 0.001	41	0.002	0.003	0.002	0.002	< 0.001	< 0.001
8	0.989	0.989	0.989	0.986	< 0.001	< 0.001	42	0.998	1.000	0.999	0.998	1.000	0.682
9	0.793	0.774	0.724	0.793	0.296	0.005	45	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.001
10	1.000	1.000	0.999	1.000	< 0.001	< 0.001	46	0.991	0.989	0.992	0.991	0.930	0.626
12	0.069	0.069	0.497	0.023	0.053	< 0.001	47	0.507	0.724	0.668	0.504	0.027	0.008
13	0.011	0.001	0.052	0.005	< 0.001	< 0.001	48	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.700
14	0.015	0.015	0.033	0.015	< 0.001	0.035	49	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
15	0.709	0.705	0.611	0.709	0.802	0.615	50	0.967	0.964	0.975	0.967	0.961	0.001
16	0.798	0.797	0.713	0.798	0.940	0.699	51	0.930	0.941	0.966	0.930	0.997	0.088
17	0.661	0.668	0.741	0.661	0.239	0.737	53	0.032	0.066	0.011	0.032	0.034	0.005
18	0.396	0.427	0.805	0.599	0.784	0.999	55	0.323	0.242	0.470	0.323	0.624	0.281
19	0.993	0.993	0.988	0.993	0.990	0.978	56	0.295	0.137	0.916	0.295	0.852	0.001
20	0.032	0.021	0.124	0.032	0.007	0.067	57	0.053	0.035	0.163	0.053	0.297	0.003
21	0.280	0.357	1.000	0.280	0.992	< 0.001	58	0.136	0.120	0.715	0.136	0.966	0.033
22	0.207	0.234	0.234	0.204	0.824	< 0.001	59	0.038	0.047	0.033	0.038	0.135	0.760
23	0.003	0.005	0.147	0.003	0.023	< 0.001	60	0.267	0.163	0.638	0.267	0.659	< 0.001
24	0.397	0.471	0.852	0.366	0.743	0.014	64	0.336	0.391	0.297	0.336	0.024	0.019
25	0.424	0.435	0.532	0.293	0.739	0.477	65	0.273	0.123	0.944	0.273	0.025	0.116
26	0.975	0.975	0.588	0.921	0.960	0.990	67	0.024	0.002	0.996	0.024	0.151	0.003
27	0.970	0.981	0.981	0.966	0.994	0.202	69	0.115	0.142	0.043	0.115	0.238	0.006
28	0.234	0.349	0.554	0.140	0.514	0.086	70	< 0.001	0.009	< 0.001	< 0.001	0.125	0.041
29	0.674	0.765	0.890	0.530	0.987	< 0.001	72	0.394	0.436	0.773	0.394	0.997	0.612
30	0.998	0.998	0.992	0.996	0.999	0.004	73	0.043	0.031	0.007	0.043	0.511	0.953
31	0.046	0.081	0.394	0.046	0.376	0.293	74	0.401	0.533	< 0.001	0.401	0.666	0.025
32	0.002	0.005	0.153	0.001	0.228	0.374	75	0.139	0.167	0.130	0.139	0.253	0.268
33	0.073	0.114	0.411	0.073	0.618	0.685	78	0.163	0.164	0.670	0.163	0.907	0.833
34	0.415	0.487	0.632	0.418	0.978	0.978	79	0.071	0.343	< 0.001	0.071	0.999	0.161
35	< 0.001	0.307	0.326	0.265	0.300	0.005	82	0.019	0.353	< 0.001	0.019	0.026	< 0.001
36	0.243	0.329	0.531	0.243	0.806	0.994	83	0.371	0.353	0.751	0.371	0.849	0.356
37	0.104	0.118	0.147	0.104	0.149	0.007	90	0.028	0.013	< 0.001	0.028	< 0.001	< 0.001
38	< 0.001	0.001	0.001	< 0.001	0.005	0.158	92	0.936	0.931	0.997	0.936	0.805	< 0.001
39	0.112	0.124	0.192	0.112	0.798	0.784							

Confidence level	ECPSSR	ECPSSR-HE	ECPSSR-HS	ECPSSR-U	Paul-Sacher	Kahoul et al.
Ionization cross section measurements $\sigma_i$						
95%	50	50	92	50	75	50
99%	75	67	92	75	92	58
All measurements $\sigma_{i,X,A}$						
95%	67	74	77	68	71	46
99%	85	83	83	85	80	57
All measurements $\sigma_{i,X,A}$ , excluding high energy data						
95%	69	75	86	69	70	48
99%	83	81	91	83	80	56

# Categorical analysis

95% CL for not rejecting the null hypothesis

$\chi^2$ test outcome	ECPSSR exp. $\sigma_{i,X,A}$	ECPSSR-HS exp. $\sigma_{i,X,A}$
Pass	44	55
Fail	20	9
p-value Fisher test	0.034	
p-value Pearson $\chi^2$	0.020	
p-value Yates $\chi^2$	0.035	

$\chi^2$ test outcome	Kahoul et al. exp. $\sigma_{i,X,A}$	ECPSSR-HS exp. $\sigma_{i,X,A}$
Pass	30	50
Fail	35	15
p-value Fisher test	0.001	
p-value Pearson $\chi^2$	< 0.001	
p-value Yates $\chi^2$	0.001	

## Contingency tables

- Fisher test
- $\chi^2$  with Yates correction
- Pearson  $\chi^2$  (where applicable)

## Results

**ECPSSR with Hartree-Slater correction best for K shell cross sections at low energy**

**ECPSSR OK at intermediate energy**

**High energy: scarce measurements**

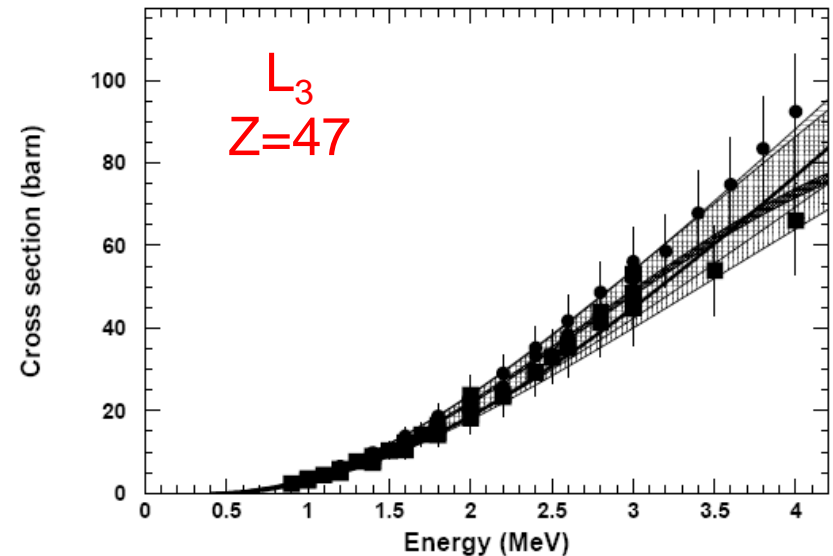
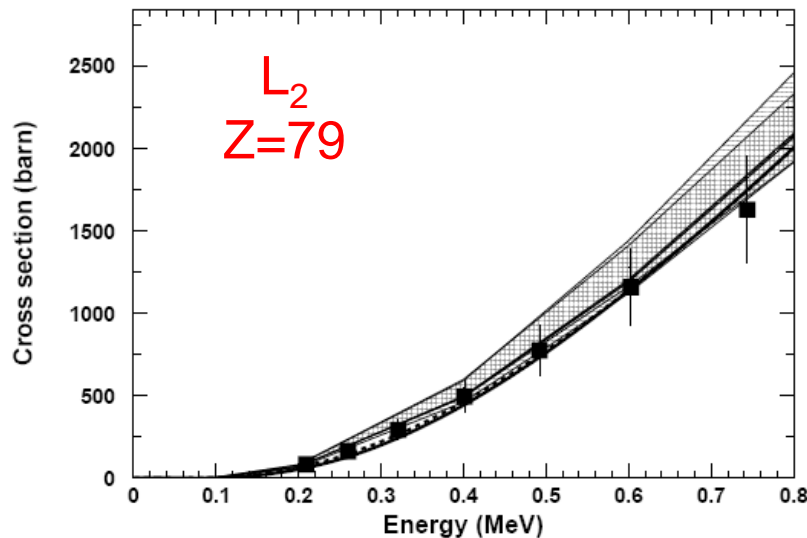
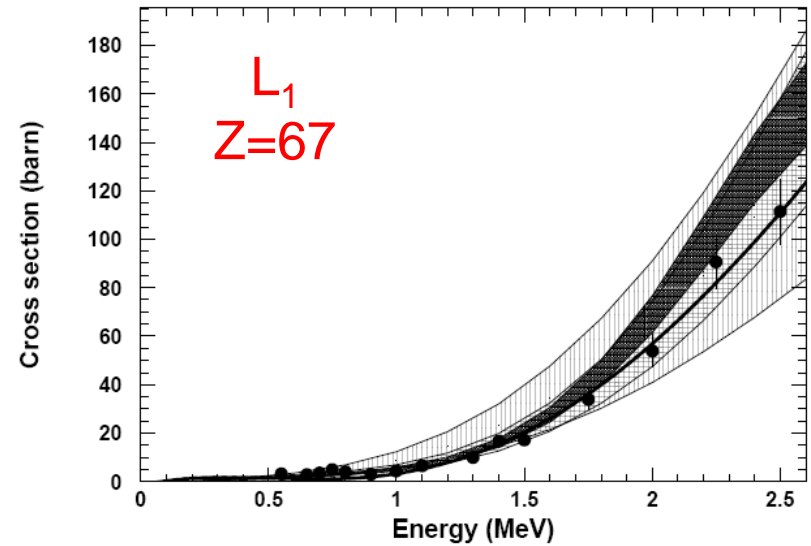
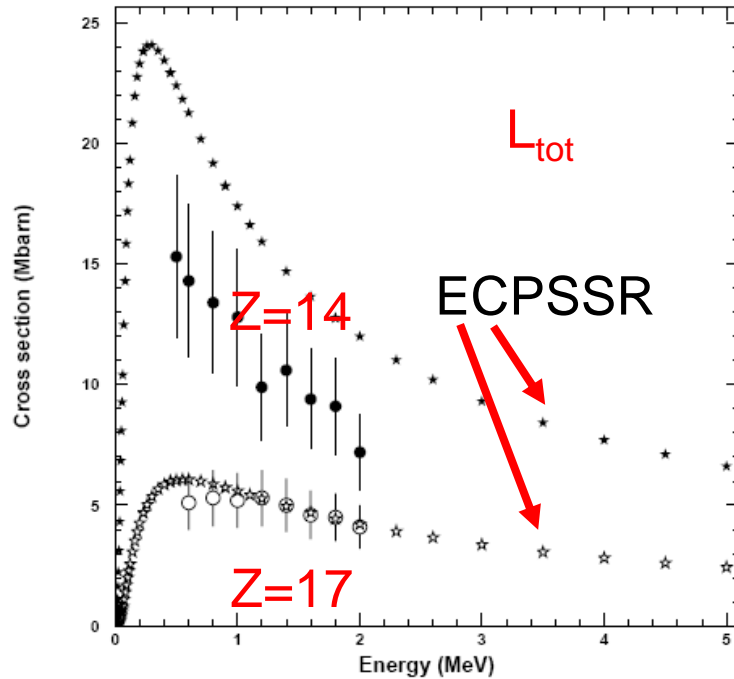
*based on objective, quantitative analysis*<sub>6</sub>



# Same validation process for L shell

## Experimental data

Compilations by  
Sokhi & Crumpton  
Orlic, Sow & Tang



# $\chi^2$ test: p-values

Z	Miyagawa et al.			Orlic et al.			Sow et al.		
	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>
45	< 0.001	0.995	0.993	< 0.001	0.005	0.004	< 0.001	0.005	0.006
46	< 0.001	0.965	0.997	< 0.001	0.003	0.003	< 0.001	0.003	0.004
47	< 0.001	0.993	0.999	0.411	0.990	0.993	0.800	0.990	0.994
48	0.904	0.995	0.999	0.679	1.000	0.998	0.648	1.000	1.000
49	< 0.001	0.987	0.975	0.838	0.992	0.981	0.621	0.993	0.989
50	< 0.001	< 0.001	0.001	0.045	1.000	1.000			
51	< 0.001	0.901	0.974	0.455	< 0.001	0.894			
52	< 0.001	0.004	0.072	< 0.001	< 0.001	0.019			
59	0.302	0.006	0.698	0.016	< 0.001	0.027			
62	0.110	0.894	0.871	0.326	< 0.001	< 0.00			
65	0.196	0.294	0.728	0.839	0.235	0.001			
66	< 0.001	< 0.001	< 0.001	0.513	0.049	< 0.00			
67	0.029	0.016	0.694	< 0.001	0.126	0.142			
70	0.015	0.999	0.602	0.979	0.999	< 0.00			
72	< 0.001	1.000	1.000	0.014	1.000	1.000			
73	< 0.001	0.753	0.988	0.253	0.213	0.952			
74	< 0.001	0.998	0.988	< 0.001	1.000	0.947			
75	0.001	1.000	0.985	0.987	1.000	0.998			
76	< 0.001	1.000	< 0.001	0.043	1.000	< 0.00			
77	< 0.001	0.764	0.849	< 0.001	0.965	0.979			
78	< 0.001	0.999	< 0.001	< 0.001	0.999	< 0.00			
79	0.021	1.000	1.000	< 0.001	1.000	1.000			
81	0.001	0.661	0.116	< 0.001	0.188	< 0.00			
82	0.356	1.000	1.000	0.005	1.000	1.000			
83	0.193	0.174	0.782	0.523	0.061	0.738			
90	0.714	0.732	0.476	0.014	0.918	0.158			
92	< 0.001	< 0.001	0.133	< 0.001	< 0.001	0.005			

Z	ECPSSR			ECPSSR-UA		
	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>
45	0.030	0.001	0.229	0.004	0.055	0.986
46	0.607	< 0.001	0.059	0.539	0.008	0.822
47	0.966	0.014	0.423	0.952	0.133	0.965
48	0.846	0.101	0.938	0.856	0.282	0.998
49	0.068	0.078	0.667	0.088	0.246	0.975
50	0.208	0.088	0.215	0.131	0.158	0.136
51	0.944	1.000	0.997	0.972	1.000	0.998
52	0.515	0.714	0.472	0.460	0.717	0.406
59	0.051	0.344	0.018	0.093	0.662	0.384
62	0.980	0.004	0.080	0.977	0.055	0.747
64	0.029	< 0.001	0.761	0.011	< 0.001	0.284
65	0.967	< 0.001	0.292	0.987	< 0.001	0.909
66	0.949	0.836	0.643	0.951	0.863	0.506
67	0.261	0.146	0.587	0.261	0.320	0.894
70	0.598	0.128	0.574	0.598	0.137	0.991
72	0.974	1.000	1.000	0.974	1.000	1.000
73	0.941	0.059	0.520	0.941	0.124	0.864
74	< 0.001	0.340	0.941	< 0.001	0.451	0.926
75	0.979	0.400	0.963	0.979	0.458	0.964
76	0.029	0.592	< 0.001	0.029	0.738	< 0.001
77	< 0.001	0.326	1.000	< 0.001	0.428	0.981
78	< 0.001	0.993	< 0.001	< 0.001	0.995	< 0.001
79	0.914	1.000	1.000	0.914	1.000	1.000
81	< 0.001	0.017	0.057	< 0.001	0.017	0.104
82	< 0.001	0.837	1.000	< 0.001	0.839	1.000
83	0.079	0.312	0.459	0.079	0.312	0.508
90	0.004	0.048	0.961	0.004	0.048	0.993
92	< 0.001	< 0.001	0.089	< 0.001	< 0.001	0.022

Contingency tables

# Results for L shell

Miyagawa et al. empirical model		
$\chi^2$ test outcome	ECPSSR-UA	Miyagawa et al.
Pass	65	51
Fail	19	30
p-value Fisher test	0.060	
p-value Pearson $\chi^2$	0.043	
p-value Yates $\chi^2$	0.063	
Orlic et al. semi-empirical model		
$\chi^2$ test outcome	ECPSSR-UA	Orlic et al.
Pass	65	45
Fail	19	36
p-value Fisher test	0.005	
p-value Pearson $\chi^2$	0.003	
p-value Yates $\chi^2$	0.005	
Sow et al. empirical model		
$\chi^2$ test outcome	ECPSSR-UA	Sow et al.
Pass	65	60
Fail	19	21
p-value Fisher test	0.717	
p-value Pearson $\chi^2$	0.620	
p-value Yates $\chi^2$	0.754	
ECPSSR original formulation		
$\chi^2$ test outcome	ECPSSR-UA	ECPSSR
Pass	65	62
Fail	19	22
p-value Fisher test	0.720	
p-value Pearson $\chi^2$	0.590	
p-value Yates $\chi^2$	0.719	

ECPSSR			
Confidence level	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>
95%	64	68	89
99%	75	79	93
ECPSSR United Atom			
Confidence level	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>
95%	64	79	89
99%	71	86	93
Miyagawa et al.			
Confidence level	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>
95%	26	78	85
99%	37	81	85
Orlic et al.			
Confidence level	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>
95%	41	70	56
99%	37	81	85
Sow et al.			
Confidence level	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>
95%	56	85	81
99%	70	85	85

**ECPSSR - United Atom**  
**best compatibility with**  
**experimental data**

**ECPSSR OK**

**Orlic et al.:** worst compatibility  
with experimental data

# M shell

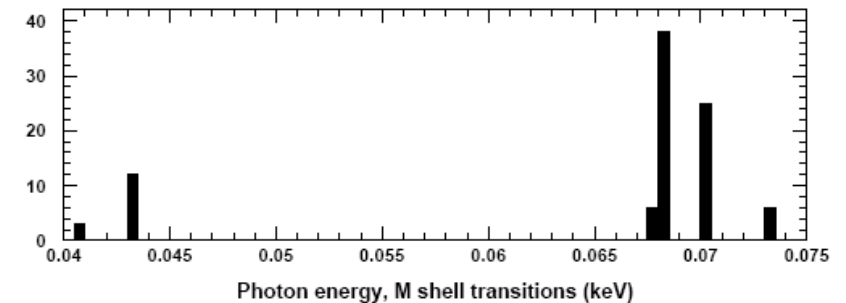
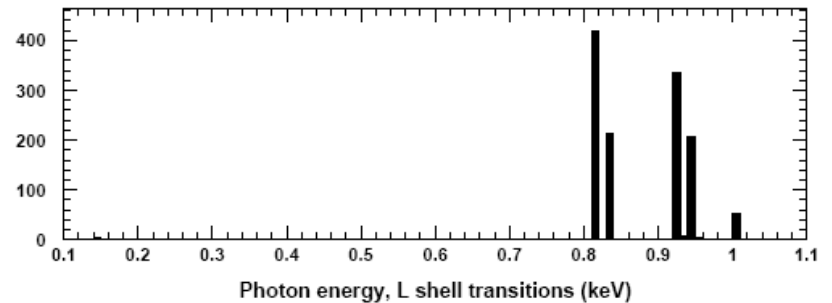
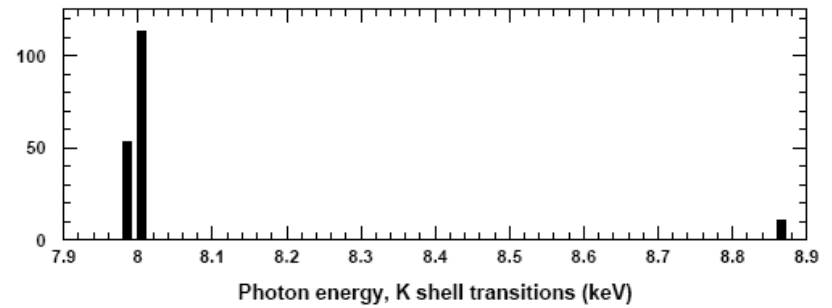
- The same analysis will be performed once there are any experimental data...

# Geant4 atomic relaxation

Geant4 simulation based on **EADL**

Validation of **X-ray energies**  
against Des Lattes et al.  
experimental review compilation

Thorough study of theoretical  
models of **emission rates** against  
experimental data



IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 3, JUNE 2007

Geant4 Atomic Relaxation

2007

Susanna Guatelli, Alfonso Mantero, Barbara Mascialino, Petteri Nieminen, and Maria Grazia Pia

594

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 3, JUNE 2007

Validation of Geant4 Atomic Relaxation Against the  
NIST Physical Reference Data

2007

S. Guatelli, A. Mantero, B. Mascialino, M. G. Pia, and V. Zampichelli

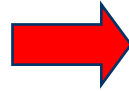
Maria Grazia Pia, *INFN Genova*

M.G. Pia and M. Sudhakar *under review*

Evaluation of radiative emission rates calculations<sub>1</sub>

# So, are all the problems solved?

Determination of a  
**vacancy**



Relative probability of  
ionising a shell w.r.t. the  
other shells

But we **do not know** the total ionisation cross section  
*(without introducing a dependency on cuts)*

We can calculate ionisation cross sections only for **K, L, M** shells

OK for light elements

Overestimate inner shell vacancies for heavier elements

Known, controllable limitation

*In principle, the issue would be solved if we could calculate  
ionisation cross sections for all shells*

# So, would all the problems be solved?

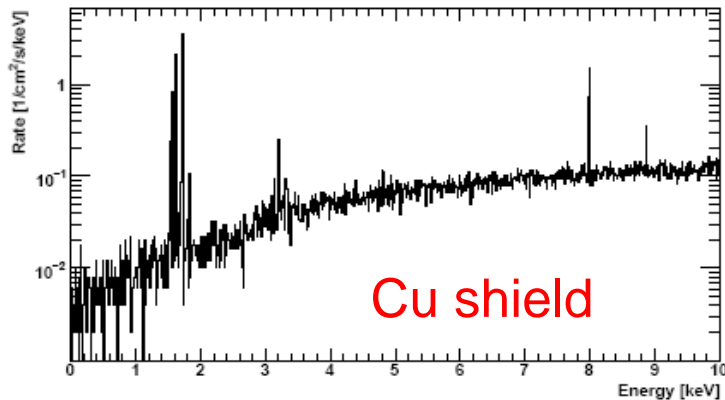
- **PIXE** (i.e. creation of a vacancy) **is still associated with the discrete treatment of continuous-discrete ionisation**
  - Indirect dependence on cuts
- **Ionisation cross section calculation for outer shells**
  - No existing theoretical calculations (*except a PWBA attempt on N shell*)
  - Hardly any experimental data
  - Long and complex calculations, with assumptions and approximations
- **$\delta$ -ray emission and ionised shell are not related**

We are in better shape than with previous Geant4

**But there is still a long way to go...**

The current R&D models can be used for **real-life experimental studies** (*knowing their limitations*)

Average Pixel Energy Spectrum 1<sup>st</sup> PIXE spectra ever produced with Geant4!

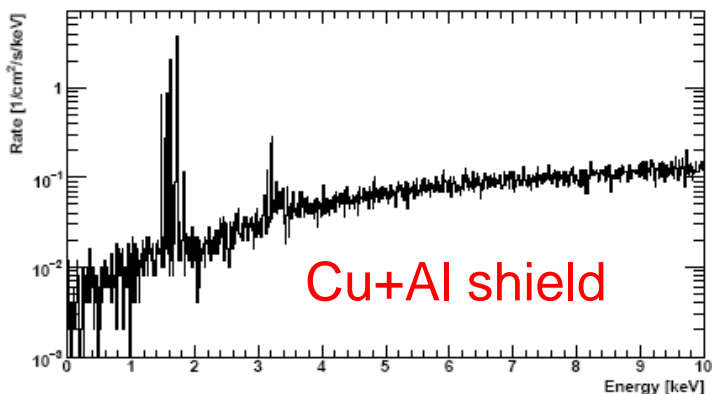


## Experimental application

Optimisation of the shielding of the X-ray detectors

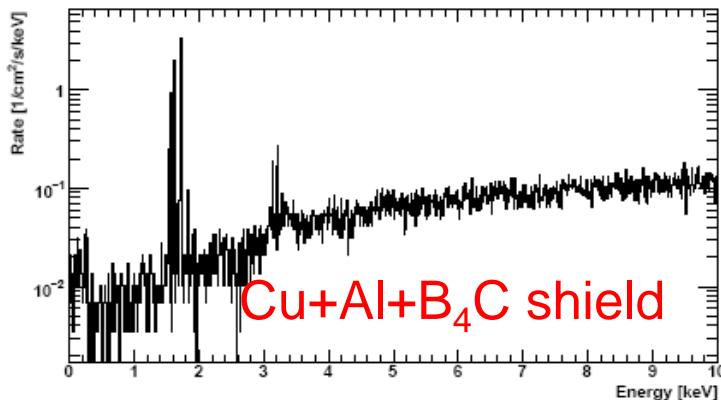
eROSITA telescope  
on the Spectrum-X-gamma  
space mission

Average Pixel Energy Spectrum



The R&D software is adequate for experimental applications concerned with **relative effects of experimentally relevant spectra**

Average Pixel Energy Spectrum



But **absolute calculations** are still out of reach for heavier elements (involving outer shells than M)





## R&D on co-working transport schemes in Geant4

- **Project launched at INFN (2009), international-multidisciplinary team**
  - **R&D** = research **study**, exploration of novel ideas
  - Distinct from Geant4 **production service**: no perturbation to running experiments!
  - R&D deliverable(s) = prototypes [to be evaluated for transition into Geant4 releases]
- **Scientific motivation**
  - From concrete experimental use cases
- **Objective**
  - Seamless transition of simulation régime in Geant4
  - Capability of simulating complex multi-scale systems
- **Conceptual and software design challenges**
  - Physics process adaptation to environment
  - Embedding “mutability” in Monte Carlo physics entities
- **Difficult**
  - ...not yet present in any simulation system

**Would all the problems be solved?  
We don't know it yet...**



# Nuclear Science Symposium Medical Imaging Conference

25-31 October 2009 • Orlando, Florida, USA

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- Instrumentation for Homeland Security
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- Neutron Imaging and Radiography
- New Detector Concepts and Instrumentation
- Nuclear Measurements and Monitoring Techniques
- Nuclear Physics Instrumentation
- Nuclear Power
- Photodetectors and Scintillation Detectors
- Radiation Damage Effects